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The Tuning of Resonances in the Generalized Random Trimer Model

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Abstract

The existence of nonscattered states in random systems of trimers in its generalized form and a base element is studied in the context of a tight binding Hamiltonian. Many conditions for the existence of such states in this generalized random trimer model (GRTM) are obtained by introducing appropriate structural correlations between the host element and the trimer. This aspect of the correlated disorder systems was not studied before. The condition for tuning the positions of the two sets of nonscattered states is obtained. We further show that the two resonances of a single trimer in the host lattice can be merged at a single energy. For this case, when the resonance energy is inside the host band, the width of the nonscattered states is found to decay as $\sim N^{-1/4}$. N is the number of sites in the system. This is a novel result. To our knowledge, this is the first time such a result is obtained. Experiments to observe the broadening of the width are proposed. In all other cases width is shown to decay as $\sim N^{-1/2}$.

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I. INTRODUCTION

One of the well established results[1-4] in condensed matter physics is that all electronic eigenstates of a disordered one dimensional system are exponentially localized irrespective of the strength of the disorder. The early work of Anderson[1] on uncorrelated site-diagonal disorder in the tight binding model (TBM) and of Mott and Twose[3] form the basis of this result. Of course, the result of Anderson, and Mott and Twose cannot be rigorously valid in one dimensional systems in which the disorder is correlated. For example, in the context of a TBM it has been shown that correlated off-diagonal disorder cannot localize the state at the band center.[5,6] Another example in this category is the model proposed by Dunlap, Kundu and Phillips (DKP).[7] Disorder in the DKP model arises from the dilation of the lattice. The coupling of the electronic motion to the structure induced disorder is described by a tight binding Hamiltonian (TBH) in which disorder appears both in the diagonal and the off-diagonal terms. Once a specific correlation between the diagonal and the off-diagonal disorder is postulated, one obtains a set of nonscattered states. The most well known example, however, is the random dimer model (RDM).[8-12] This is basically the off-spring of the original DKP model. RDMs are random binary alloys with elements of one component appearing in pairs. So, in the context of a TBH, this model is characterized by a short range correlation in site energies. Due to this short range correlation, a set of nonscattered states in the neighborhood of the dimer energy is obtained. The obvious generalization of the RDM is, of course, random n-mer model[12] in which the length of the correlation in site energies is increased beyond the nearest sites. So, a random n-mer model is a random alloy of a distinct host element and a cluster of 'n' number of elements. All of these n elements may or may not be same. But, some of these must be distinct from the host element. If the cluster contains only one type of element, the random n-mer model ($n > 2$) is then expected to sustain nonscattered states at more than one energy, provided certain constraints are met. This is precisely so. Recently Sil *etal*[13] have shown that those energies can be found from the zeros of the n-th Chebysev polynomial of second kind. The argument of the Chebysev polynomial

is the trace of the transfer matrix of the element of the cluster. Furthermore, if the cluster contains elements in even numbers and has a plane of symmetry, it can be converted to a dimer by a real space renormalization group (RSRG)[14] procedure. By converting such clusters to dimers it has been shown that a binary random system of such clusters and a host element can sustain nonscattered states. Other studies[12,14–16] involve the changing of the hopping elements inside the cluster without destroying the plane of symmetry. Even with this generalization, nonscattered states have been obtained. The repulsive binary alloy (RBA)[16] and the magnon problem[5,6] are two such examples. We note that the cluster in the RBA contains three elements, two of which are host sites. This cluster also has a plane of symmetry. Hence, RBA can also be transformed to an effective random dimer system.

The total transparency of the cluster in the neighborhood of an energy belonging to the band of the host system is due to the vanishing of scattering of the incoming wave due to the cluster. Consequently, a set of nonscattered states is obtained around that energy in the random system of the cluster of interest and the host unit. In as much as the presence of the nonscattered states in random systems can give rise to the anomalous transport properties, a systematic investigation of the resonance property of the clusters of various sizes and kinds is, therefore, necessary. For example, the maximum number of resonances that a one dimensional n–site cluster can yield is $(n-1)$. Hence, it is necessary to find out the conditions for obtaining these resonances. The effect of these resonances on the widths of the nonscattered states also needs to be studied. Furthermore, a cluster with more than two sites can yield more than one resonance. Therefore, in trimers and larger clusters it is possible to obtain condition(s) for two or more resonances to merge at a single energy. If such a situation is obtained, the width of the nonscattered states will increase substantially. Consequently, a profound change in the transport properties will be observed. Since a trimer is the simplest possible cluster which can exhibit all these properties, we plan to study in this paper the resonance property of a trimer in its generalized form. The random system of the trimer in its generalized form and a host site will be referred to as the Generalized random trimer model (GRTM). Of course, we assume that GRTM can be described by an appropriate

TBH. Note that the well known random trimer model (RTM) and the RBA are two spec cases of this generalized version. Furthermore, the results for the RDM can also be obtain from this general model. Hence, GRTM encompasses many hitherto known models. show in this paper that GRTM can yield many conditions for obtaining nonscattered sta provided appropriate structural correlations between the host element and the element the trimer are introduced. Consequently, this model may be applied to physical syste in which structural correlations play crucial roles. Moreover, there are conditions for whi GRTM yields two sets of nonscattered states due to the additional structural correlatio If these two energies are close to each other, states in between these energies develope ve large localization length. Another interesting feature of this model is that the positions the resonances can be adjusted by modulating the site-energy of the central atom of th trimer. Of course, the trimer should possess a plane of symmetry. In the extreme cas these two resonances can be merged at a single energy. To our knowledge we are the firs to obtain this interesting result. These results can be verified by fabricating appropri layered heterojunction and by coupling quantum dots.[17] Furthermore, the degeneracy resonances that we encounter here may be the key to the understanding of the anomalo elctrical conductivity in polyaniline and other related systems.

The organization of this paper is as folllows. In Sec.II, we present the relevant aspects GRTM and calculate the transmission coefficient of a system containing only a single trim in its general form. In Sec.III, we present the arguments for the presence of nonscatter states in GRTM. We calculate the number of nonscattered states using our method.[10] Th pole structure behavior of the site Green function is studied. This is necessary to understan the nature of the nonscattered states at the band edges of the host system. We conclu the paper by highlighting the features that differentiate GRTM from the well known RDM

II. TRANSMISSION COEFFICIENT FOR A SINGLE GENERALIZED TRIMER

As mentioned earlier we are dealing with a random binary system made up of a host element and cluster of three elements which are different from the host element. We further assume that the static and the dynamical properties of the system can be described adequately by a TBH with nearest-neighbor hopping only. We assign ϵ_a, ϵ_b and ϵ_c to the site energies in the cluster (ABC). Without any loss of generality we set zero to the site-energy of the host element. In other words, site energies in the cluster are measured relative to the site energy of the host system. We assume that the nearest neighbor hopping terms in the cluster are V_0. All other nearest neighbor hopping terms that will appear in the system are given the same value, say unity. So, the effect of off-diagonal disorder on the energy states are treated in a limited way in our model.

Our aim is to find the energies at which the random system sustains nonscattered states. To find those energies it is necessary to find the energies at which a single cluster embedded in the host lattice is transparent. Following Liu and Chao[18] the transmision coefficient ($|T|^2$) of the single cluster is calculated. In as much as the calculation is very standard, we only present below the relevant results.

$$|T|^2 = \frac{4-\omega^2}{A^2+B^2+C^2+D^2+(A-D)(B-C)\omega - AD\omega^2+2}, \tag{1}$$

where

$$A = \frac{(\omega-\epsilon_a)(\omega-\epsilon_b)(\omega-\epsilon_c)}{V_0^2} - (2\omega-\epsilon_a-\epsilon_c),$$
$$B = 1 - \frac{(\omega-\epsilon_c)(\omega-\epsilon_b)}{V_0^2},$$
$$C = \frac{(\omega-\epsilon_b)(\omega-\epsilon_a)}{V_0^2} - 1,$$
$$D = -\frac{(\omega-\epsilon_b)}{V_0^2}.$$

Furthermore, ω is the particle energy which is $2\cos k$. k is the wave vector. We now discuss the various cases.

Case I: $\epsilon_a = \epsilon_b$, $\epsilon_c = 0$

In this case we obtain $|T|^2 = 1$ at $\omega = \epsilon_a$, when $V_0 = 1$. This is the usual dimer case.[10]

Case II: $\epsilon_a = \epsilon_c = 0$, $\epsilon_b = (1-V_0^2)\omega_0$.

This cluster yields $|T|^2 = 1$ at ω_0 with the constraint $|\omega_0| \leq 2$. This is the RBA case.[16]

Case III: $\epsilon_a = \epsilon_b = \epsilon_c = \epsilon_0$.

This case yields two values of the particle energy ω, namely ω_+ and ω_-, at which $|T|^2 = 1$. They are

$$\omega_+ = \epsilon_0 + V_0 e^{\xi} \tag{2a}$$

and

$$\omega_- = \epsilon_0 - V_0 e^{-\xi}, \tag{2b}$$

where the parameter ξ is defined by

$$\sinh\xi = \frac{1-V_0^2}{2V_0\epsilon_0}.$$

We also need $|\omega_\pm| \leq 2$. When $V_0 = 1$, the cluster is refered to as a trimer.[12] For this case we obtain $|T|^2 = 1$ at $\omega = \epsilon_0 \pm 1$, provided $|\epsilon_0| \leq 1$. On the other hand for $1 < |\epsilon_0| \leq 3$, we obtain $|T|^2 = 1$ at a single energy. If $|\epsilon_0| > 3$, $|T|^2$ will not yield unity at any permissible value of ω.

Case IV: $\epsilon_b = \epsilon_a + \epsilon_c$

This system yields $|T|^2 = 1$ at $\omega = \epsilon_b$ for any value of V_0. Of course, we need $|\epsilon_b| \leq 2$. However, ϵ_a and ϵ_c may take any value provided the required constraint is met. Note that the symmetry[12] in the defect cluster is not necessary for the vanishing of the reflection coefficient. We also find that for a particular value of V_0, the width of the transmission peak becomes sharper as the values of $|\epsilon_a|$ and $|\epsilon_c|$ are increased. Due to the constraint, there is a ladder in the site energies around the central element of the trimer. As we increase the magnitude of $|\epsilon_a|$ and $|\epsilon_c|$, the situation becomes more and more similar to the Stark localization of Bloch eigenstates in a pure crystal by a strong applied electric field.[19] Hence, the width of the transmission peak should decrease. Similarly, if we reduce V_0 keeping ϵ_a

and ϵ_c fixed, we reduce the overlap between site Wannier orbitals. Consequently, the width of the transmission peak will decrease. Conversely, increasing V_0, we allow the electron to see the cluster in a mean field way. This, inturn, increases the width of the transmision zone. These are actually observed and presented in Fig. 1. We should also point out that the site energy of the central unit also depends on the site energy of the host unit. Hence, there is a structural correlation between the trimer and the host. In the dimer, trimer, and the RBA, this kind of structural correlation is also present. It appears through the ineqalities which are required to be satisfied by the relevant site-energies. This correlation for these cases is, however, weak.

Case V: $\epsilon_a = \epsilon_c = \epsilon_s$ and $\epsilon_b = \epsilon_0$

This is basically the generalized version of RBA. This is, however, a ternary system. Since the reflection coefficient $|R|^2$ will be zero at the perfect resonance, resonance energies are calculated by setting the numerator of the expression for $|R|^2$ to zero. Consequently, a second order algebraic equation in ω is obtained.

$$\omega^2 - [\epsilon_0 + \epsilon_s + \frac{1-V_0^2}{\epsilon_s}]\omega + (\epsilon_0\epsilon_s - 2V_0^2 + \frac{\epsilon_0}{\epsilon_s}) = 0. \tag{3}$$

The two roots ($\omega_\pm$) of this equations are

$$\omega_\pm = \epsilon_s + \frac{1}{2}[p \pm \sqrt{p^2 - 4q}], \tag{4}$$

where

$$p = \epsilon_0 - \epsilon_s + \frac{1-V_0^2}{\epsilon_s},$$
$$q = \frac{\epsilon_0}{\epsilon_s} - (1+V_0^2).$$

To obtain $|T|^2 = 1$ at $\omega_\pm$, these two roots must satisfy two conditions, namely (i) $|\omega_\pm| \leq 2$ and (ii) $\omega_\pm$ must be real. The reality of $\omega_\pm$ requires $p^2 \geq 4q$. Since RBA and RTM are special cases of this situation, results for those cases can also be obtained from $\omega_\pm$. Note that when $q = 0$, we have

$$\epsilon_0 = (1+V_0^2)\epsilon_s. \tag{5}$$

With this choice we obtain $|T|^2 = 1$ at $\omega_- = \epsilon_s$ and $\omega_+ = \epsilon_0 + (1-V_0^2)\frac{1}{\epsilon_s}$. It is apparent that for any choice of V_0 and $|\epsilon_s| \leq 2$, ω_+ may not belong to [-2, 2]. Furthermore, for $V_0 = 1$, two resonances appear exactly at site energies of the trimer, namely ϵ_0 and $\frac{\epsilon_0}{2}$. The general expression of $\omega_\pm$ also suggests that two resonances can be brought closer together by changing the ratio $\frac{\epsilon_0}{\epsilon_s}$. This shows the importance of the structural correlation. The condition for the two resonances to merge at a single energy yields

$$\epsilon_0 = \frac{[\epsilon_s^2 + 1 + V_0^2 - 2|V_0|\sqrt{1-\epsilon_s^2}]}{\epsilon_s}. \tag{6}$$

Since ϵ_0 must be a real quantity, the inequality $|\epsilon_s| \leq 1$ must be satisfied. As a special case if we introduce Eq. (5) in Eq. (6) we find that two resonances will merge exactly at ϵ_s provided $V_0^2 = (1-\epsilon_s^2)^{-1}$. So, if the trimer contains a plane of symmetry, the positions of the resonances can be tuned by modulating the central energy of the trimer in the prescribed way. This is the major result of this paper.

III. NONSCATTERED STATES IN GRTM

In as much as a single trimer embeded in a host system is totally transparent at certain energies depending on the structure of the trimer, it is natural to ask whether or not a random system of these trimers and the host is also transparent at those energies. In the case of RDM, this is found to be so.[10] It has also been claimed that the RBA and the random trimer system are also totally transparent at the resonance energies of the system with a single cluster.[12,16] We, therefore, present here the numerical calculation of the transmission coefficient of those random systems which form the base of this paper. The cases considered are: (a) $\epsilon_b = \epsilon_a + \epsilon_c$, $V_0 = 1$, (b) $\epsilon_a = \epsilon_c = \epsilon_s$, $\epsilon_b = \epsilon_0 = (1+V_0^2)\epsilon_s$, (c) $\epsilon_a = \epsilon_c = \frac{\epsilon_b}{2}$, $\epsilon_b = \epsilon_0$ and (d) $\epsilon_b = \frac{[\epsilon_s^2+1+V_0^2-2|V_0|\sqrt{1-\epsilon_s^2}]}{\epsilon_s}$. The results are presented in Figs. 2(a)-2(d). The procedure of Datta, Giri and Kundu[10] is employed to obtain these results. The salient features of these calculations are as follows.

(i) The additional structural correlation introduced in these models is not sufficient to

suppress the overwhelming localization tendency of most of the states due to the substitutional disorder.

(ii) The random systems also yield unity for the transmission coefficient ($|T(\omega)|^2$) at the resonance energies of the single trimer system.

(iii) For a given length (N) of the random system, the transmission coefficient at the energies between two resonance energies depends strongly on the separation of the resonance energies. Compare Fig. 2(c) and Fig. 3.

(iv) For a given N, the width of the transmitting zone for the case where two resonances merge is subtantially larger than the width of the transmitting zone of a comparable random dimer system.[10]

(v) If we take $\epsilon_s = 1$ and $V_0 = 1$, for the case (d) two resonances appear at $\omega_0 = 2.0$, i.e at the upper band edge of the host system. We find that compared to the random dimer case, the width of the transmitting zone shown in Fig. 4 is substantially large.[10]

We now show by an analytical method[20] that the random systems under consideration sustain in general extended states at the energies (say ω_0) at which the transmission coefficient is unity. The proof goes as follows. Let $t_3(\omega)$ and $t_p(\omega)$ be the transfer matrix of the trimer and the perfect site respectively.

$$t_3(\omega) = \begin{bmatrix} A(\omega) & B(\omega) \\ C(\omega) & D(\omega) \end{bmatrix}. \tag{7}$$

with A, B, C and D already defined in the previous section and

$$t_p(\omega) = \begin{bmatrix} \omega & -1 \\ 1 & 0 \end{bmatrix}. \tag{8}$$

For t_3 and t_p to commute at a certain energy, say ω_0, we need

$$B = -C, \tag{9}$$

and

$$A - D = C\omega_0. \tag{10}$$

If ω_0 denotes the resonance energy for the single trimer system, the form of $t_3(\omega_0)$ for various cases discussed in the previous section are as follows.

Case I.

$$\epsilon_a = \epsilon_b, \quad \epsilon_c = 0.$$

$$t_3(\epsilon_a) = -t_p(\epsilon_a) \text{ at } \omega_0 = \epsilon_a.$$

Case II.

$$\epsilon_a = \epsilon_c = 0, \ \epsilon_a = (1 - V_0^2)\,\omega_0, |\,\omega_0\,| \leq 2$$

$$t_3(\omega_0) = t_p^3(\omega_0).$$

Case III.

$$\epsilon_a = \epsilon_b = \epsilon_c = \epsilon_0, \ V_0 = 1$$

$$t_3(\omega_0) = \pm I \text{ at } \omega_0 = \epsilon_0 \pm 1.$$

However, if $V_0 \neq 1$, t_3 does not reduce either to a unit matrix or t_p. But it can be shown that t_3 and t_p commute with each other at the resonance energies.

Case IV.

$$\epsilon_b = \epsilon_a + \epsilon_c$$

$$t_3(\epsilon_b) = t_p(\epsilon_b) \text{ at } \omega_0 = \epsilon_b.$$

Case V : $\epsilon_a = \epsilon_c = \epsilon_s$

In this general case, t_3 does not always reduce to a simple recognizable form as in the other cases. However, at the resonance energies t_3 indeed commutes with t_p. For the special cases namely, (i) $\epsilon_b = \epsilon_0$, $\epsilon_s = \frac{\epsilon_0}{2}$, $V_0 = 1$, $|\,\epsilon_0\,| \leq 2$ and (ii) $\epsilon_b = \epsilon_0 = (1 + V_0^2)\epsilon_s$, $|\,\epsilon_s\,| \leq 2$, the form of t_3 at the resonance energies are

$$(i) \ t_3(\epsilon_0) = t_p(\epsilon_0),$$

$$t_3(\frac{\epsilon_0}{2}) = t_p^{-1}(\frac{\epsilon_0}{2}),$$

and

$$(ii)\ \ t_3(\epsilon_s) = t_p^{-1}(\epsilon_s)$$

respectively. According to Wu, Goff and Phillips[12] the sufficient condition for a random system of this type to sustain a nonscattered states at ω_0 is that the cluster transfer matrix must reduce to either a unit matrix or that of a perfect site. Here, we constructed examples for which such a situation is not obtained. It is, therefore, necessary to prove that the state at ω_0 in all these cases is in general extended.

Since t_3 and t_p commute with each other at ω_0 for all these cases, Furstenberg's theorem[20,21] cannot be applied here to discern the nature of the state at ω_0. To determine the nature of the state at ω_0 we need to solve explicitly the Fourier transform of the amplitude $(C_n(\omega))$ at each site. In the transfer matrix formalism[18,22] the amplitude at the $n-th$ site is related to the amplitude at the given sites by

$$X_{n+1} = T_n X_1, \tag{11}$$

when $X_n^T = (C_{n+1}(\omega), C_n(\omega))$. T_n, which is called the transfer matrix, is a random product of t_3 and t_p for the cases under study. Since both t_3 and t_p are unimodular matrices irrespective of ω, T_n is also a unimodular matrix. Furthermore, T_n is a 2×2 matrix. Hence, the two eigenvalues (λ_1, λ_2) of T_n can be written as e^{θ} and $e^{-\theta}$. θ is either real or purely imaginary. Consequently, the trace of T_n $(= 2\cosh\theta)$ is a real quantity. This is true for all n and ω. Now suppose that a string of N sites contain m_1 trimer and $m_2 = (N-3m_1)$ host sites. Since t_3 and t_p commute at ω_0, at this energy we have

$$T_N(\omega_0) = [t_3(\omega_0)]^{m_1}[t_p(\omega_0)]^{N-3m_1}. \tag{12}$$

In as much as two diagonalizable commuting matrices can be simultaneously diagonalized, we assume that U is such a matrix which diagonalizes both $t_3(\omega_0)$ and $t_p(\omega_0)$. If the eigenvalues of $t_3(\omega_0)$ and $t_p(\omega_0)$ are $e^{\pm\phi_3}$ and $e^{\pm\phi_p}$ respectively, we have

$$U^{-1}T_N(\omega)U = \begin{bmatrix} a & 0 \\ 0 & a^{-1} \end{bmatrix}, \tag{13}$$

where $a = \exp[m_1\phi_3 + (N-3m_1)\phi_p]$. Furthermore, we have

$$\mathrm{Tr}[T_N(\omega_0)] = 2\cosh[m_1\phi_3 + (N-3m_1)\phi_p]. \tag{14}$$

Assume now that $\omega_0 = 2\cos k_0$. Since trace of $t_p(\omega_0)$ is bounded by 2, two eigenvalues o t_p will be purely imaginary. In other words ϕ_p will be purely imaginary. It can be show that $\phi_p = ik_0$. Now, if ϕ_3 is real at ω_0, the trace of $T_N(\omega_0)$ will be a complex quantity a ω_0. This is a contradiction. So, the trace of $t_3(\omega_0)$ should be bounded by 2. It can be easil verified for all the cases considered here that the trace of $t_3(\omega_0)$ is indeed bounded by 2. Th important consequence of this result is that the trace of $T_N(\omega_0)$ is also bounded by 2. Thi can also be verified numerically. We should emphasize that $|\ \mathrm{Tr}T_N(\omega_0)\ | \leq 2$ is a necessar condition for the state at ω_0 to be extended.

Because of the commutation of t_3 and t_p at ω_0, the calculation of $C_{N+1}(\omega_0)$ and $C_N(\omega_0$ is trivial. So, we present the result only.

$$C_{N+1}(\omega_0) = \frac{\sin(\theta + k_0)}{\sin k_0}C_1 - \frac{\sin\theta}{\sin k_0}C_0, \tag{15a}$$

and

$$C_N(\omega_0) = \frac{\sin\theta}{\sin k_0}C_1 - \frac{\sin(\theta - k_0)}{\sin k_0}C_0. \tag{15b}$$

Here $\theta = m_1\phi_3 + (N-3m_1)k_0$. C_1 and C_0 are given initial condition. Since ϕ_3 is a mod$(2\pi$ quantity, as long as ω_0 is inside the host band, both C_{N+1} and C_N are bounded. Hence,

$$\lim_{N\to\infty}\frac{1}{N}[C_{N+1}^2 + C_N^2] \to 0. \tag{16}$$

Consequently, the state at ω_0 cannot be exponentially localized. Furthermore, due to th boundedness of $C_N(\omega_0)$ and $C_{N+1}(\omega_0)$, the solution of the amplitude equation at ω_0 canno grow. Therefore, the state at ω_0 should be extended in nature as long as ω_0 is inside th host band.

However, for all the cases considered here when the resonance is appearing at the ban edges of the host system, we find a pole in the Green function[10,23] of the host system with trimer impurity. We present our result in Fig. 5 for the case of degenerate resonances. Sin

the Green function shows a pole, the state at the band edges cannot be extended. Of course, it will not be exponentially localized because condition (16) will be still satisfied. We argue by analogy with the random dimer system that the state at the band edges are algebraically localized.[10] We plan to check this proposition by the band width scaling method in our future work.

To determine the nature of the states in the vicinity of ω_0 we assume that the total transmission coefficient $| T_N(\omega) |^2$ when ω is in the vicinity of ω_0 is approximately[10]

$$| T_N(\omega) |^2 \simeq | t_s(\omega) |^{2m_1} . \tag{17}$$

Here, m_1 is the number of trimers in the sample. $| t_s(\omega) |^2$ and $| r_s(\omega) |^2$ are the transmission and reflection coefficient of a single trimer at ω respectively. In this approximation we neglect the effect of multiple back scattering of the incident particle for $\omega \sim \omega_0$. Furthermore, we assume that there exists a value of N beyond which two resonances are well separated. Consequently, they can be treated independently. Since $| t_s(\omega) |^2 + | r_s(\omega) |^2 = 1$, Eq. (17) can be written as

$$| T_N(\omega) |^2 \simeq e^{-\rho N \sum_{n=1}^{\infty} | r_s(\omega) |^{2n} / n} , \tag{18}$$

with $\rho = m_1/N$. It is easy to see that if $| r_s(\omega) |^2 < \frac{1}{N}$, $| T_N(\omega) |^2 \to 1$ as $N \to \infty$. To find the energy width we first note that our numerical calculations show that for $\omega \sim \omega_0$, $| r_s(\omega) |^2 \sim 0$. So, we expand $| r_s(\omega) |^2$ in Taylor's series around ω_0 which is a zero of $| r_s(\omega) |^2$. Furthermore, for $| \omega_0 | < 2$, the absolute minimum of $| r_s(\omega) |^2$ also occurs at ω_0. Therefore, if $| \omega_0 | < 2$, in the leading order approximation we must have

$$| r_s(\omega) |^2 \sim a_2(\omega - \omega_0)^2, \tag{19}$$

where $a_2 = \frac{\partial^2 |r_s(\omega)|^2}{\partial \omega^2} |_{\omega=\omega_0}$ and a_2 should be positive definite. Consequently, around ω_0 we obtain

$$| T_N(\omega) |^2 \simeq e^{-\rho a_2 (\omega - \omega_0)^2 N}. \tag{20}$$

So, from this derivation we find that the inverse localization length of the states in the neighborhood of ω_0 is given by $\sim \rho a_2 (\omega - \omega_0)^2$. This in turn gives that the energy width inside which the localization length of the states is superior to the sample size is approximately $\frac{1}{\sqrt{N}}$. Since $\omega = 2 \cos k$, for $k \sim k_0$ we have

$$(\omega - \omega_0)^2 \sim 4 \sin^2 k_0 \, | \Delta k |^2 . \tag{21}$$

So, if we assume that Bloch k's are good quantum number in the vicinity of ω_0, we then obtain approximately $\sqrt{N}$ Bloch type extended states for each resonance.

When two resonances merge at a single energy we find that

$$| r_s(\omega) |^2 \simeq a_4 (\omega - \omega_0)^4 \tag{22}$$

for ω_0 inside the host band and

$$| r_s(\omega) |^2 \simeq a_3 (\omega - \omega_0)^3 \tag{23}$$

if ω_0 is at one of the band edges of the host system. To understand the origin of the fourth order term in the first case we note that for a given V_0 and $\frac{\epsilon_0}{\epsilon_s}$ we obtain two energies where $| r_s(\omega) |^2$ is zero. In between these two zeros, we must have a maximum. Keeping V_0 fixed if we change $\frac{\epsilon_0}{\epsilon_s}$, two minima and the maximum move close to each other. At the critical values of $\frac{\epsilon_0}{\epsilon_s}$, these minima and the maximum merge at a single point (Fig. 6). Consequently, both the first and the second derivatives of $| r_s(\omega) |^2$ with respect to ω evaluated at ω_0 are zero. Furthermore, the function is itself zero at ω_0. Again the absolute minimum of the function occurs at ω_0 for ω_0 inside the band. Furthermore, $| r_s(\omega) |^2$ is a positive semidefinite function for $| \omega | \leq 2$. Hence, the Taylor's expansion of $| r_s(\omega) |^2$ for ω_0 inside the band should start with the fourth power in $(\omega - \omega_0)$ and a_4 must be a positive definite quantity. This can be verified by numerical calculations. The situation at the band edge is, however, different from the first case. For this case at the critical value of $\frac{\epsilon_0}{\epsilon_s}$ we also observe the coalescence of a maximum and a minimum at the band edge of interest (Fig. 7). But, the resonance energy is not the absolute minimum of $| r_s(\omega) |^2$. This can be seen from the analytical continuation of

$| r_s(\omega) |^2$ for $| \omega | > 2$ (Inset of Fig. 7). Hence, the leading term of the Taylor's expansion in this case should start with $(\omega - \omega_0)^3$. Furthermore, the positive semidefiniteness of $| r_s(\omega) |^2$ for $| \omega | \leq 2$ demands that a_3 should always be negitive definite at the upper band edge and positive definite at the lower band edge.

If we now apply similar analysis as before, we find that the width of nonscattered states goes as $\sim N^{-1/4}$ for ω_0 inside the host band. So, the number of Bloch type extended states will be approximately $N^{3/4}$. On the other hand the width of the totally transmitting zone goes as $N^{-1/3}$ if ω_0 is at the band edge of the host system. Although the present calculation of the width of the nonscattered states is an approximate one, qualitatively correct results were obtained by this method in the case of RDM.[10] Since the cases where resonances do not merge are very similar to the random dimer case, we believe that results obtained from the present analysis are qualitatively correct. Of course, a thorough analysis of such a width and the nature of the states inside the width is desired. This will be presented elsewhere.

IV. CONCLUSION

A dimer being the simplest possible cluster does not offer any scope to improve upon the width of the nonscattered states. It is, therefore, necessary to find random systems which are simple but at the same time offer the opportunity to increase the width of the nonscattered states by adjusting a few relevant parameters. If this can be done, random systems will show enhanced electrical conductivity at low temperatures. Trimers in this respect are found to be ideal in many ways. The structure of a trimer is not very complicated. Consequently, it does not contain many adjustable parameters. Hence, it is possible to fabricate these trimers to study their resonance property. For example, strained layers of Ge-Si alloy of different compositon or Si can be grown on Ge to obtain adjustable potential wells.[24] So, equivalent trimer systems can be prepared. Furthermore, symmetric trimers offer the opportunity to tune the positions of the resonances. In the extreme case two resonances can be merged at a single energy. This interesting feature of symmetric trimers makes them extremely

worthy of experimental ivestigations. It also remains to be seen whether this interesting feature of symmetric trimers has any role to play in the anomalous electrical conductivity in polyanilines and other related materials. This work is in progress.

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FIGURES

FIG. 1. Plot of transmission coefficient ($|T|^2$) as a function of particle energy for Case IV. (a) $\epsilon_a = -3$, $\epsilon_c = 3$, $V_0 = 0.8$ (Solid line). (b) $\epsilon_a = -1$, $\epsilon_c = 1$, $V_0 = 0.8$ (Dashed line). (c) $\epsilon_a = -1$, $\epsilon_c = 1$, $V_0 = 4$ (Dot-Dashed line).

FIG. 2. Plot of transmission coefficient ($|T|^2$) as a function of particle energy for the random segment of length $N = 10^4$ for different conditions. (a)$\epsilon_b = \epsilon_a + \epsilon_c, V_0 = 1$; here, $\epsilon_a = 0.6$, $\epsilon_c = 0.4$. (b) $\epsilon_a = \epsilon_c = \epsilon_s, \epsilon_b = \epsilon_0 = (1 + V_0^2)\epsilon_s$; here, $\epsilon_s = 1.1$, $V_0 = 0.8$. (c) $\epsilon_a = \epsilon_c = \epsilon_b/2, \epsilon_b = \epsilon_0$ and $V_0 = 1$; for this case $\epsilon_0 = 1.0$. (d) $\epsilon_0 = \frac{\epsilon_s^2+1+V_0^2-2|V_0|(1-\epsilon_s^2)^{1/2}}{\epsilon_s}$ with $\epsilon_s = 0.5$ and $V_0 = 1$.

FIG. 3. Same as Fig. 2(c), but $\epsilon_0 = 1.8$ and $V_0 = 1$.

FIG. 4. Same as Fig. 2(d), but $\epsilon_s = 1.0$ and $V_0 = 1$.

FIG. 5. Solid and dashed curve corresponding to the real and imaginary part of the Green function (G) with impurity ϵ_b and ϵ_c calculated at site a as a function of particle energy. The solid straight line corresponds to $G = \frac{1}{\epsilon_a}$. Here, $\epsilon_a = \epsilon_c = 0.5$ and $V_0 = 1$.

FIG. 6. Plot of reflection coefficient as a function of particle energy for the single cluster in the host system for various values of ϵ_0/ϵ_s with $\epsilon_s = 0.5$ (fixed) and $V_0 = 1$. Here, two resonances will be inside the band. (a) $\frac{\epsilon_0}{\epsilon_s} = 2.4$ (Dashed line); (b) $\frac{\epsilon_0}{\epsilon_s} = 9 - 4\,(3^{0.5})$ (Solid line); this is the case where two resonances merge at a single energy; (c) $\frac{\epsilon_0}{\epsilon_s} = 1.8$ (Dot-Dashed line); (d) $\frac{\epsilon_0}{\epsilon_s} = 1.2$ (Dot line).

FIG. 7. Same as Fig. 6, but here at least one resonance will be at the band edge. Value of $\epsilon_s = 1.0$ (fixed) and $V_0 = 1$. (a) $\frac{\epsilon_0}{\epsilon_s} = 3.0$ (Solid line). Here, two resonances merge at a single energy (Band edge); (b) $\frac{\epsilon_0}{\epsilon_s} = 2$ (Dashed line); (c) $\frac{\epsilon_0}{\epsilon_s} = 1.5$ (Dot-Dashed line); (d) $\frac{\epsilon_0}{\epsilon_s} = 1.0$ (Dot line). Inset shows the analytical continuation of $|r_s(\omega)|^2$ of Case (a) for $\omega > 2$.

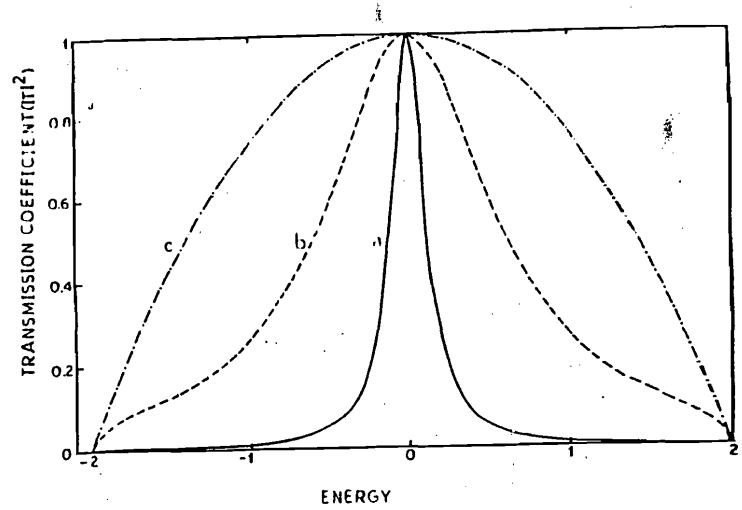


Fig.1

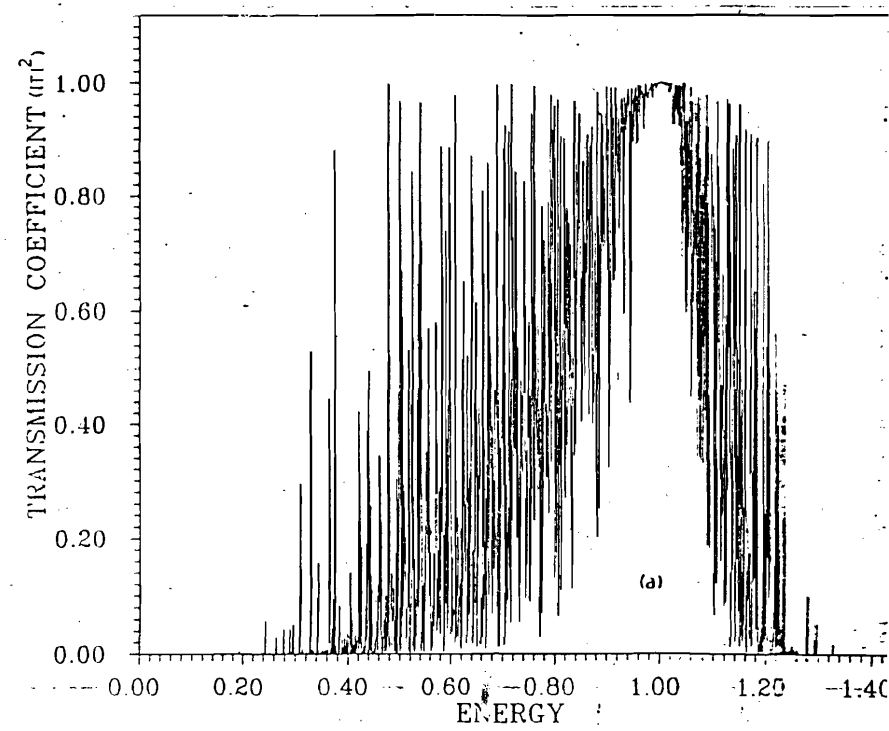
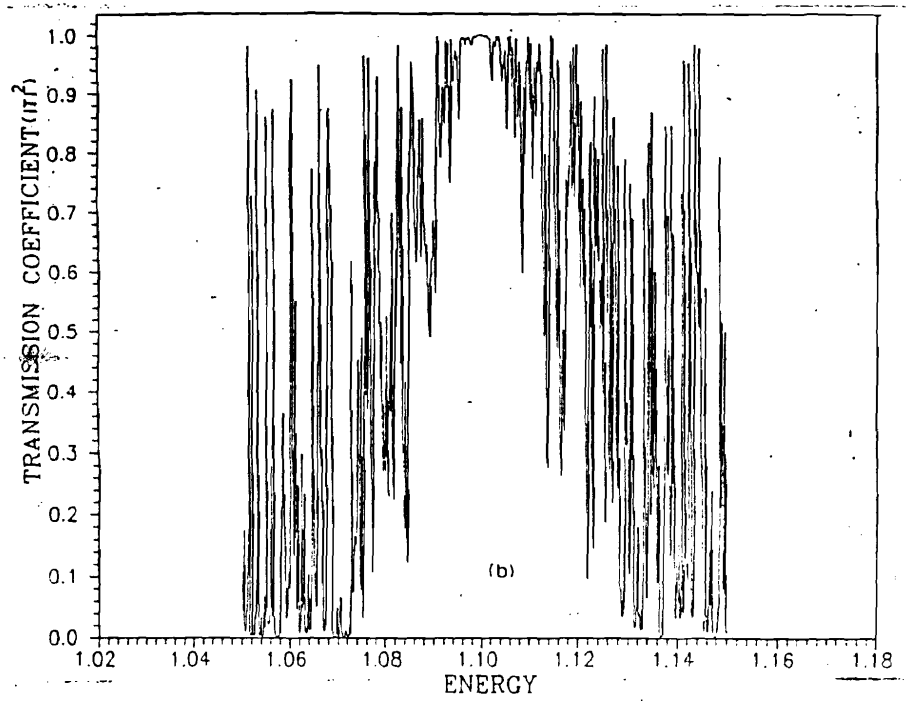


Fig.2



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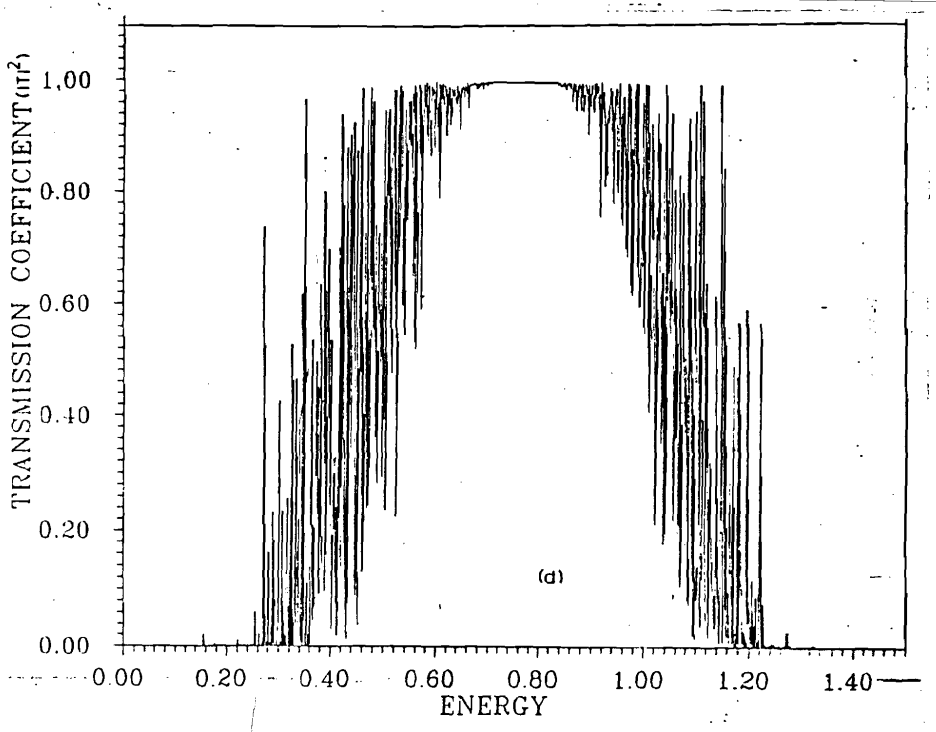

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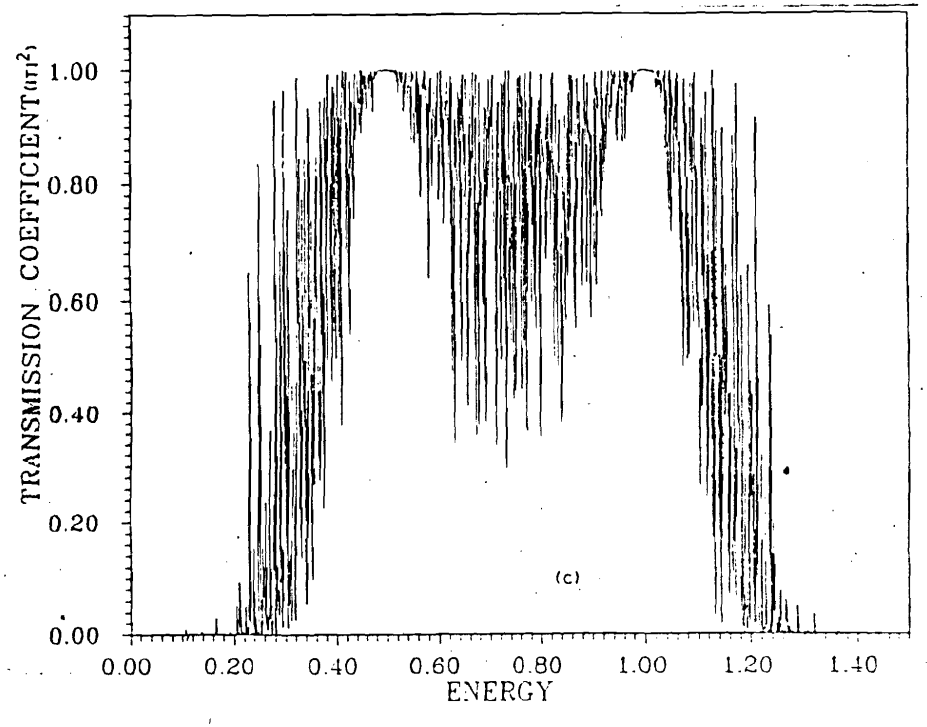

Fig 2

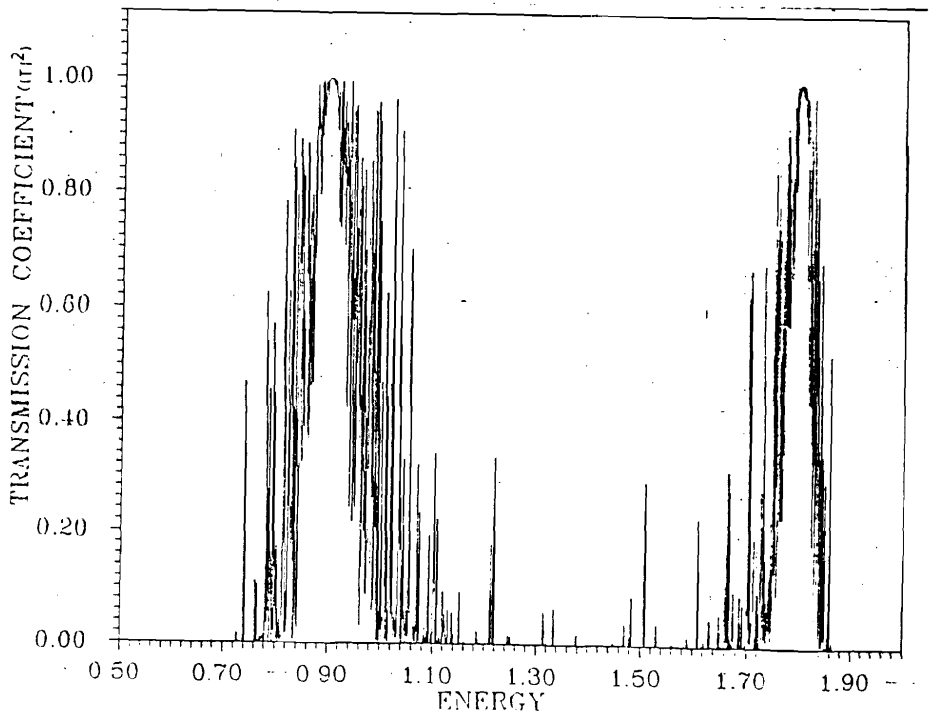

Fig-3

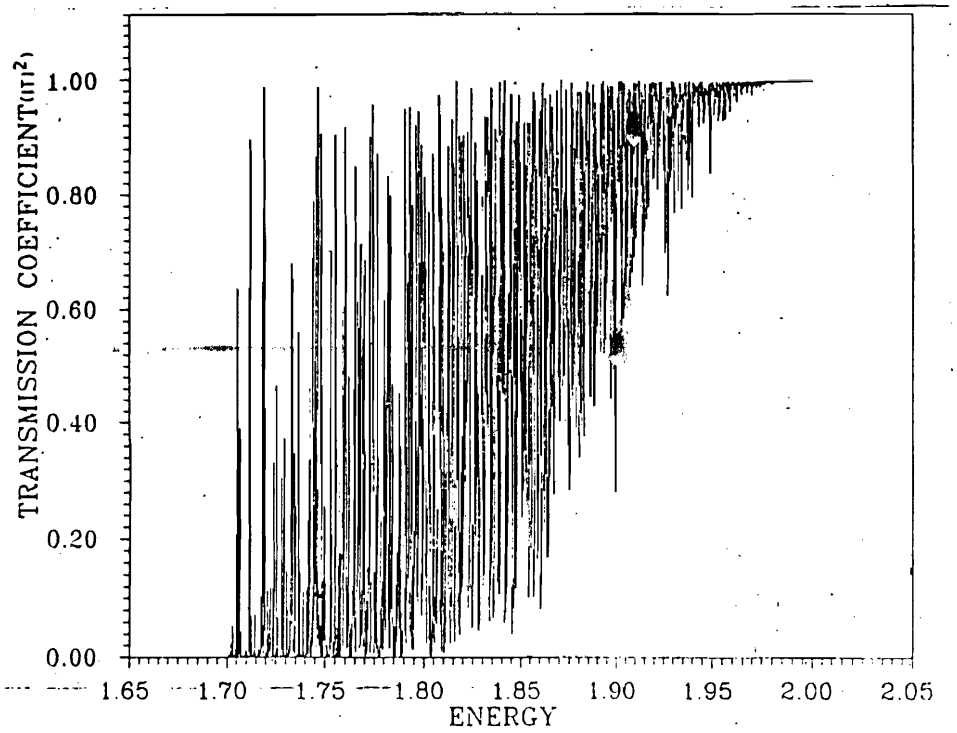

Fig.4

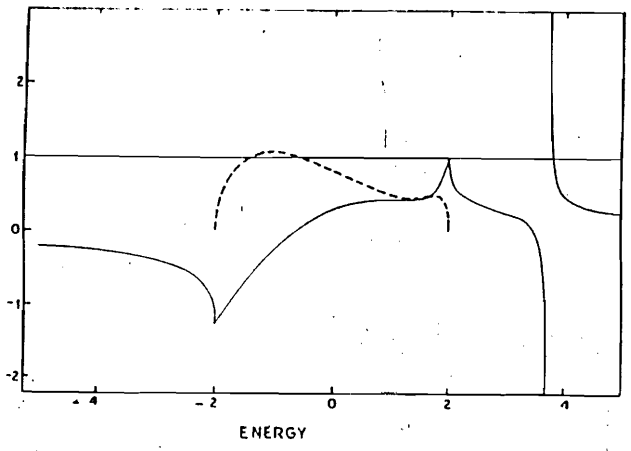

Fig.5

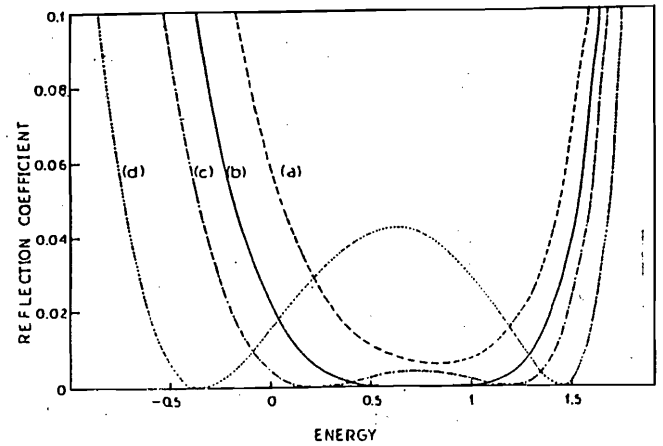

Fig.6

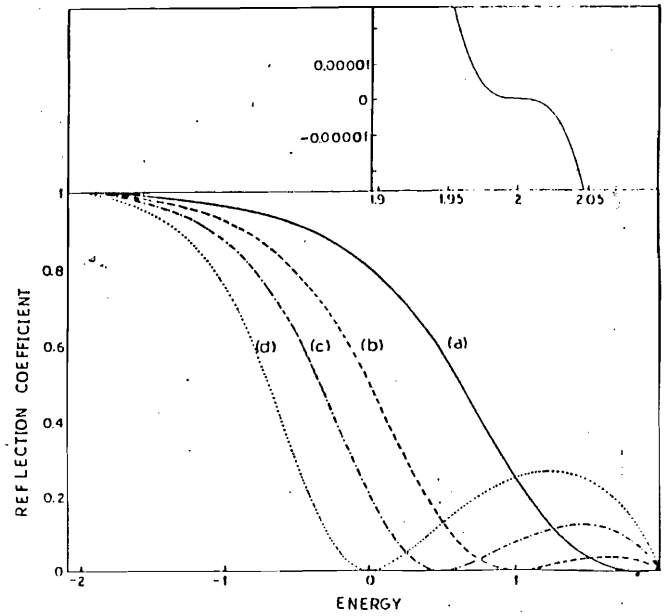

Fig.7